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Microscopic Optical-Model Analysis of Electron Scattering from Atomic Hydrogen*

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The projection-operator formalism advanced by Feshbach is used to derive a numerically tractable equation which describes the elastic scattering of electrons from atomic hydrogen under multichannel conditions. By neglecting the potential of interaction in the inverse operator, analytical expressions can be obtained for the Green's function which permit the inclusion of both discrete and continuum target-state contributions to the optical potential. The numerical procedures used to solve the resulting nonlocal integrodifferential equation and to generate differential, total elastic and inelastic cross sections are discussed. Good agreement is found with available experimental data.

I. INTRODUCTION

The theoretical determination of atomic and molecular scattering cross sections in the low-energy region is greatly complicated by the presence of a large (usually infinite) number of open scattering channels. Thus, in order to obtain an accurate description of scattering phenomena for charged particles of energy below the region where the Born approximation is valid, effects due to the various inelastic processes which may occur must be included. The usual practice of expanding the total wave functions in terms of a set of target eigenfunctions leads to an infinite set of coupled differential equations which describe the scattering probabilities for elastic and inelastic processes. The difficulties associated with large coupled sets of equations preclude accurate solutions for all but a very limited range of projectile energies.[1]

Two important effects that should be accounted for at low energies in electron scattering from atoms and molecules are exchange and polarization. Exchange arises as a result of the Pauli principle and is accounted for by explicitly antisymmetrizing the electronic wave functions. Polarization is the distortion of the electronic wave functions in the presence of the incident projectile resulting in virtual excitations which contribute to the elastic scattering amplitude. The target electrons are often assumed to adjust adiabatically at low projectile energies though dynamic polarization effects are operative at the lowest projectile energies.[2–5] The adiabatic assumption is expected to be very inappropriate for atoms such as the alkali-earth metals in which polarization effects are expected to be large. The microscopic optical model described by Feshbach[6,7] and Bell and Squires[8] is formulated directly from the exact, nonrelativistic, many-body Schrödinger equation. The dynamical properties of the interaction are an integral part of the formalism.

Feshbach developed an elegant and powerful technique for determining elastic and inelastic scattering cross sections under multichannel conditions. In the projection-operator approach the total wave function, which describes the interacting system, is projected onto the elastic channel subspace and all other channels are included in a complex nonlocal "optical-potential" operator. The difficulties associated with a large set of coupled equations are transformed into the complexities associated with the optical potential. However, the formalism is amenable to a number of different approximations which offer some distinct advantages over other methods of calculating cross sections in the difficult low-energy region.

The optical-potential formalism has been applied to a number of different atomic and molecular scattering problems. Mittleman and Watson first formally applied the concepts of the optical model to the scattering of slow electrons from hydrogen.[2] The Feshbach projection-operator formulation of the optical potential was first applied by Hahn, O'Malley, and Spruch to atomic scattering of electrons and positrons for single-channel scattering.[9] The formal developments of Feshbach were applied by Chen to slow-electron scattering by molecules. The results of this study illustrate the role of compound negative-ion states in the vibrational excitation of molecules.[10] A theoretical treatment of dissociative attachment of electrons to diatomic molecules was made by O'Malley using the projection-operator formalism.[11] The technique was also used by Rotenberg to describe elastic scattering of an atom from a structureless rigid rotator.[12]

In the present investigation, we have utilized optical-potential analysis to determine atomic scattering cross sections in the energy region where inelastic processes are important but below where the Born approximation is applicable. With this method it is possible to investigate the importance of various inelastic contributions and total scattering cross sections without encountering the difficulties associated with large sets of coupled differential equations.

The basic Feshbach formalism is briefly outlined in Sec. II. Our particular choice of a Green's function for electron-hydrogen scattering and the resulting elastic channel radial equations are described in Secs. III and IV. A brief description of the numerical procedures which were used in solving the complex nonlocal radial equations is given in Sec. V, followed by results and conclusions in Sec. VI.

II. FORMALISM

The wave function χ that describes a quantum-mechanical system with definite symmetry properties can be expanded in any complete basis set of eigenfunctions which span the same space. Introducing such an expansion into the Schrödinger equation leads to an infinite set of coupled differential equations, which can be manipulated into a single equation by using the Feshbach approach.

The Schrödinger equation, describing the interaction between a projectile and a structured target, is

$$(E_t - H)\chi = 0 \ , \tag{1}$$

where E_t and H are the total energy and Hamiltonian of the system. We define a projection operator P which projects onto the elastic channel subspace of the total Hilbert space spanned by the eigenfunctions of H. We also define a complementary projection operator $Q = 1 - P$ which projects onto the complete inelastic channel subspace. By using the properties of P and Q, we can transform Eq. (1) into two coupled equations

$$(E_t - PHP)P\chi = (PHQ)Q\chi \tag{2}$$

and

$$(E_t - QHQ)Q\chi = (QHP)P\chi \ . \tag{3}$$

Formally, we can solve Eq. (3) for $Q\chi$ and substitute the result into Eq. (2) to obtain

$$[PHP + PHQ(E_t^+ - QHQ)^{-1}QHP - E_t]\,P\chi = 0 \ . \tag{4}$$

Equation (4) is an integrodifferential equation whose solution $P\chi$ represents the elastic channel component of the total wave function χ for the system. The complex, nonlocal operator $PHQ(E_t^+ - QHQ)^{-1}\,QHP$ is referred to as the "optical potential." In Eq. (4) $E_t^+ = E_t + i\delta$ for outgoing waves, δ being a positive infinitesimal. PHQ and QHP in Eq. (4) represent interactions between two complementary segments of the Hilbert space which is spanned by P and Q.

III. APPROXIMATIONS TO THE GREEN'S FUNCTION

The Green's function which describes the interaction between a target with one internal coordinate $\vec{r}$ and a projectile at position $\vec{R}$ with respect to the center of mass of the target is the solution to

$$(E_t^+ - QHQ)G(\vec{R},\vec{R}';\vec{r},\vec{r}') = \delta(\vec{R}-\vec{R}')\delta(\vec{r}-\vec{r}') . \qquad (5)$$

We may solve Eq. (5) formally for G:

$$G(\vec{R},\vec{R}';\vec{r},\vec{r}') = (E_t^+ - QHQ)^{-1}\delta(\vec{R}-\vec{R}')\delta(\vec{r}-\vec{r}') . \qquad (6)$$

Denoting the eigenfunctions of $(E_t^+ - QHQ)^{-1}$ by $|\varphi_i(\vec{R},\vec{r})\rangle$, we use the closure relation

$$\delta(\vec{R}-\vec{R}')\delta(\vec{r}-\vec{r}') = \sum_i |\varphi_i(\vec{R},\vec{r})\rangle\langle\varphi_i(\vec{R}',\vec{r}')| \qquad (7)$$

to write

$$G(\vec{R},\vec{R}';\vec{r},\vec{r}') = \sum_i \frac{|\varphi_i(\vec{R},\vec{r})\rangle\langle\varphi_i(\vec{R}',\vec{r}')|}{E_t - \xi_i} \qquad (8)$$

for the Green's function which describes a bound final state of the projectile and

$$G^+(\vec{R},\vec{R}';\vec{r},\vec{r}') = \lim_{\delta\to 0}(2\pi)^{-3} \times\int_C d\vec{k}\, \frac{|\varphi_k(\vec{R},\vec{r})\rangle\langle\varphi_k(\vec{R}',\vec{r}')|}{E_t + i\delta - \xi_k} \qquad (9)$$

for the continuum final states of the projectile where ξ_i and ξ_k are eigenvalues belonging to the eigenfunctions φ. The contour C in expression (9) is chosen to satisfy the boundary condition at infinity for outgoing waves. The basis functions are chosen to be solutions to the equation

$$(QHQ - \xi)\,|\varphi(\vec{R},\vec{r})\rangle = 0 . \qquad (10)$$

In practice, the solution to Eq. (10) is formidable. However, the equation is amenable to a number of approximations. For example, we may choose only the diagonal components of QHQ or replace the potential function in QHQ by a local function. In these approximations the Green's functions may be expressed as

$$G(\vec{R},\vec{R}';\vec{r},\vec{r}') = \sum_i \frac{|\chi_i(\vec{R})\rangle\langle\chi_i(\vec{R}')|\,Q_i}{E_t - \epsilon_i - \xi_i'} , \qquad (11)$$

$$G^+(\vec{R},\vec{R}';\vec{r},\vec{r}') = \lim_{\delta\to 0}\frac{1}{(2\pi)^3} \times\int_c d\vec{k}\, \frac{|\chi_i(\vec{k},\vec{R})\rangle\langle\chi_i(\vec{k},\vec{R}')|\,Q_i}{E_t + i\delta - \epsilon_i - \hbar^2k^2/2\mu_p} , \qquad (12)$$

where ξ_i' and $\hbar^2k^2/2\mu_p$ are the eigenenergies of the bound and continuum intermediate states of the projectile, respectively, and ϵ_i is the eigenenergy of the ith excited state of the target. The wave functions χ are solutions to the relative motion equations which describe the intermediate states of the projectile,

$$\left(-\frac{\hbar^2}{2\mu_p}\nabla^2 + v_{ii}(\vec{R}) - \xi_i'\right)\chi_i(\vec{R}) = 0 \qquad (13)$$

and

$$\left(-\frac{\hbar^2}{2\mu_p}\nabla^2 + v_{ii}(\vec{R}) - \frac{\hbar^2k^2}{2\mu_p}\right)\chi_i(\vec{k},\vec{R}) = 0 . \qquad (14)$$

Expressions (11) and (12) are numerically tractable. However, in problems where the continuum states of the target make important contributions to the scattering interaction, numerical determination of this part of the optical potential is not practicable with present computers.

Another approximation that may be used is one in which the potenital of interaction is neglected in the inverse operator. Analytical expressions can then be obtained for the Green's functions and numerical solutions found which include the contributions from the discrete and continuum states of the target to the optical potential. This approximation has been used by Rotenberg in a microscopic optical-model analysis of atomic scattering from a structureless rigid rotator.[12] We shall also use this approach in the present study of electron scattering from atomic hydrogen.

The open-channel Green's functions for this case are easily derived. For the energy-conserving discrete target excitations, we can write

$$G^+(\vec{R}\vec{R}';\vec{r},\vec{r}') = -\frac{\mu_p}{2\pi\hbar^2}\frac{e^{i\beta_{n'}|\vec{R}-\vec{R}'|}}{|\vec{R}-\vec{R}'|}Q_{n'} , \qquad (15)$$

where

$$\beta_{n'} = \left(\frac{2\mu_p}{\hbar^2}(E_t - \epsilon_{n'})\right)^{1/2} \quad \text{for } E_t \geq \epsilon_{n'} .$$

Here μ_p is the reduced mass of the projectile and target, $\epsilon_{n'}$ is the excitation energy of the n'th discrete state of the target, and $Q_{n'}$ is the projection operator for the n'th excited state of the target. The energy-nonconserving Green's function for the discrete target excitations is given by

$$G^+(\vec{R},\vec{R}';\vec{r},\vec{r}') = -\frac{\mu_p}{2\pi\hbar^2}\frac{e^{-\alpha_{n'}|\vec{R}-\vec{R}'|}}{|\vec{R}-\vec{R}'|}Q_{n'} , \qquad (16)$$

where

$$\alpha_{n'} = \left(\frac{2\mu_p}{\hbar^2}(\epsilon_{n'} - E_t)\right)^{1/2} \quad \text{for } \epsilon_{n'} > E_t .$$

Similarly, we write the Green's functions for the target-continuum energy-conserving transitions

$$G^+(\vec{R},\vec{R}';\vec{r},\vec{r}') = -\frac{\mu_p}{2\pi\hbar^2}\frac{e^{i\beta_c|\vec{R}-\vec{R}'|}}{|\vec{R}-\vec{R}'|}Q_c , \qquad (17)$$

where

$$\beta_c = \left(\frac{2\mu_p}{\hbar^2}\left(E_t - \frac{\hbar^2}{2m}k_1^2\right)\right)^{1/2} \quad \text{for } E_t \geq \hbar^2k_1^2/2m .$$

Here k_1 is the magnitude of the wave vector of the initially bound target electron of mass m and Q_c is the projection operator for the continuum states of the target. For the energy-nonconserving transitions

$$G^+(\vec{R}, \vec{R}'; \vec{r}, \vec{r}') = -\frac{\mu_p}{2\pi\hbar^2} \frac{e^{-\alpha_c|\vec{R}-\vec{R}'|}}{|\vec{R}-\vec{R}'|} Q_c , \tag{18}$$

where

$$\alpha_c = \left[\frac{2\mu_p}{\hbar^2}\left(\frac{\hbar^2}{2m} k_1^2 - E_t\right)\right]^{1/2} \quad \text{for } \hbar^2 k_1^2/2m > E_t .$$

The appropriate multipole expansions for terms found in the Green's function are

$$\frac{e^{i\beta|\vec{R}-\vec{R}'|}}{|\vec{R}-\vec{R}'|} = 4\pi i\beta \sum_{l=0}^{\infty} \sum_{m=-l}^{l} j_l(\beta R_<) h_l^{(1)}(\beta R_>) \times Y_{lm}(\hat{R}) Y_{lm}^*(\hat{R}') \tag{19}$$

and

$$\frac{e^{-\alpha|\vec{R}-\vec{R}'|}}{|\vec{R}-\vec{R}'|} = 8\alpha \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i_l(\alpha R_<) k_l(\alpha R_>) \times Y_{lm}(\hat{R}) Y_{lm}^*(\hat{R}') . \tag{20}$$

In expressions (19) and (20) j_l is a spherical Bessel function, $h_l^{(1)}$ is a Hankel function of the first kind, i_l and k_l are modified spherical Bessel functions as defined by Antosiewitz,[13] and Y_{lm} is a spherical harmonic. $R_>$ and $R_<$ represent the greater or lesser of the scalar quantities R and R'.

IV. DEVELOPMENT OF THE ELASTIC CHANNEL RADIAL EQUATION

The Hamiltonian of relative motion for an electron interacting with a stationary single-electron atom can be written

$$H = \left(-\frac{\hbar^2}{2\mu_p} \vec{\nabla}^2 + V(\vec{R}, \vec{r}) + H_A\right) = E_t . \tag{21}$$

In expression (21) $(-\hbar^2/2\mu_p)\vec{\nabla}^2$ is the kinetic energy operator for the relative motion of the projectile of reduced mass μ_p, $V(\vec{R}, \vec{r}) = -e^2/R + e^2/|\vec{R}-\vec{r}|$ is the potential of interaction between the electron and atom, H_A is the Hamiltonian of the isolated atom, and E_t is the total energy of the system. We choose the origin of our coordinate system to be at the center of mass of the atom and ignore exchange, spin-dependent forces, and recoil during the interaction. We confine ourselves to a particular elastic channel, allowing for excitations and ionization of the target.

We define the P projection operator as

$$P = \sum_{l_1' m_1'} |R_{nl_1'}(r) l_1' m_1'\rangle \langle R_{nl_1'}(r) l_1' m_1'| , \tag{22}$$

where $|R_{nl_1'}(r) l_1' m_1'\rangle$ is a hydrogenic wave function for any discrete state of the target with principal, orbital angular momentum, and azimuthal quantum numbers n, l_1', and m_1', respectively. We shall use the symbol $|l_1' m_1'\rangle$ to represent a spherical harmonic in the Dirac notation.

We define the Q projection operator

$$Q = 1 - P = \sum_{n'\sigma\tau} |R_{n'\sigma}(r)\sigma\tau\rangle\langle R_{n'\sigma}(r')\sigma\tau| + \frac{1}{(2\pi)^3} \sum_{\lambda\mu} \int |F_\lambda(\eta, k, r)\lambda\mu\rangle\langle F_\lambda(\eta, k_1' r')\lambda\mu| \, d\vec{k}_1' , \tag{23}$$

where all states except the set with quantum numbers n, l_1', and m_1' are to be included in the sum or integral. The $F_\lambda(\eta, k_1 r)$ are the regular Coulomb wave functions[14] which are eigenfunctions of the target Hamiltonian with continuum eigenvalues $\hbar^2 k_1^2/2m$ with the appropriate value for $\eta = -e^2 m/\hbar^2 k_1$.

To develop the elastic channel radial equation, we let $\chi_{JM}(\vec{R}, \vec{r})$ represent the total wave function for the interacting system with total angular momentum J and projection M and write

$$P\chi_{JM} = \sum_{l_1' l_2' m_1' m_2'} |R_{nl_1'}(r) l_1' m_1' l_2' m_2'\rangle \langle l_1' l_2' m_1' m_2' | JM\rangle \times \frac{U^n(l_1' l_2' J|R)}{R} . \tag{24}$$

Here $U^n(l_1' l_2' J|R)$ is the reduced wave function for the relative motion and $\langle l_1' l_2' m_1' m_2' | JM\rangle$ is a vector coupling coefficient which allows J^2 and $J_z = m_1' + m_2' = M$ to be simultaneously diagonal in the coupled representation. For a given l_1' and l_2', the values of J are restricted in the usual sense by the triangular condition

$$l_1' + l_2' \geq J \geq |l_1' - l_2'| , \tag{25}$$

where J ranges from $l_1' + l_2'$ down to $|l_1' - l_2'|$ in integral steps. It is convenient to express (22) in terms of the Wigner $3j$ symbols, so that we can take advantage of their symmetry properties[15,16]:

$$P\chi_{JM} = \sum_{l_1' l_2' m_1' m_2'} |R_{nl_1'}(r) l_1' m_1' l_2' m_2'\rangle (-1)^{l_1' - l_2' + M} \times (2J+1)^{1/2} \begin{pmatrix} l_1' & l_2' & J \\ m_1' & m_2' & -M \end{pmatrix} \frac{U^n(l_1' l_2' J|R)}{R} . \tag{26}$$

If we substitute the expressions for $P\chi$, P, Q, $G(\vec{R}, \vec{R}'; \vec{r}, \vec{r}')$, and H into Eq. (4), integrate over angular coordinates and perform a number of algebraic manipulations,[15–18] we obtain the elastic channel equation

$$\left(-\frac{\hbar^2}{2\mu_p} \frac{d^2}{dR^2} + \frac{\hbar^2}{2\mu_p} \frac{l_2(l_2+1)}{R^2} - \frac{e^2}{R} + \epsilon_n - E_t\right) U^n(l_1 l_2 J|R)$$

$$+ \sum_{l_2' l_1'' \lambda} A_{l_2' l_1' \lambda} V_{n l_1 \lambda}^{n l_1''}(R) U^n(l_1'' l_2' J|R) + \sum_{l_2' \sigma \lambda' \lambda'' l l_1'}$$

$$\times \int K^{\lambda'' l l_1'}_{l_2'\sigma\lambda'}(R,R')\,U^n(l_1'' l_2' J | R')R'\,dR' = 0 \;. \quad (27)$$

The terms appearing in Eq. (27) are defined as

$$A_{l_2' l_1'' \lambda} = [(2l_1+1)(2l_1''+1)(2l_2+1)(2l_2'+1)]^{1/2}$$

$$\times (-1)^{l_1+l_1'+J} \begin{pmatrix} l_1 & \lambda & l_1'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_1 & l_2 & J \\ l_2' & l_1'' & \lambda \end{Bmatrix} ,$$

$$K^{\lambda'' l l_1'}_{l_2'\sigma\lambda'}(R,R') = B^{\lambda'' l l_1'}_{l_2'\sigma\lambda'} \sum_{S=1}^{4} {}^{(s)}C^{\lambda'' l l_1'}_{l_2'\sigma\lambda'}(R,R') ,$$

and

$$B^{\lambda'' l l_1'}_{l_2'\sigma\lambda'} = (2\sigma+1)(2l+1)[(2l_1+1)(2l_1''+1)(2l_2+1)(2l_2'+1)]^{1/2}(-1)^{l_1+l_1'}$$

$$\times \begin{pmatrix} l_1 & \lambda' & \sigma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & \lambda' & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \sigma & \lambda'' & l_1'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & \lambda'' & l_2' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_2 & l_1 & J \\ \sigma & l & \lambda' \end{Bmatrix} \begin{Bmatrix} \sigma & l & J \\ l_2' & l_1'' & \lambda'' \end{Bmatrix} ,$$

where the expressions in curly brackets are $6j$ symbols in the Wigner notation.[15] The explicit expressions for the ${}^{(s)}C$ terms are given by

$${}^{(1)}C^{\lambda'' l l_1''}_{l_2'\sigma\lambda'}(R,R') = -\frac{2\mu_p iR}{\hbar^2} \sum_{n'=2}^{n''} \beta_{n'} V^{n'\sigma}_{nl_1\lambda'}(R)$$

$$\times j_l(\beta_{n'}R_<)h_l^{(1)}(\beta_{n'}R_>)\,V^{nl_1}_{n'\sigma\lambda''}(R') ,$$

$${}^{(2)}C^{\lambda'' l l_1''}_{l_2'\sigma\lambda'}(R,R') = -\frac{4\mu_p R}{\pi\hbar^2} \sum_{n''}^{\infty} \alpha_{n'} V^{n'\sigma}_{nl_1\lambda'}(R)$$

$$\times i_l(\alpha_{n'}R_<)k_l(\alpha_{n'}R_>)\,V^{nl_1}_{n'\sigma\lambda''}(R') ,$$

$${}^{(3)}C^{\lambda'' l l_1''}_{l_2'\sigma\lambda'}(R,R') = -\frac{4\mu_p iR}{\pi\hbar^2} \int_0^{\kappa} \beta_c k_1^2 [V^{\infty\sigma}_{nl_1\lambda'}(R)$$

$$\times j_l(\beta_c R_<)k_l^{(1)}(\beta_c R_>)V^{nl_1}_{\infty\sigma\lambda''}(R')]\,dk_1 ,$$

and

$${}^{(4)}C^{\lambda'' l l_1''}_{l_2'\sigma\lambda'}(R,R') = -\frac{8\mu_p R}{\pi^2\hbar^2} \int_{\kappa}^{\infty} \alpha_c k_1^2 \,[V^{\infty\sigma}_{nl_1\lambda'}(R)$$

$$\times i_l(\alpha_c R_<)k_l(\alpha_c R_>)V^{nl_1}_{\infty\sigma\lambda''}(R')]\,dk_1 ,$$

where

$$V^{nl_1''}_{nl_1\lambda}(R) = \left\langle R_{nl_1}(r) \right| \frac{e^2 r_<^{\lambda}}{r_>^{\lambda+1}} \left| R_{nl_1''}(r) \right\rangle ,$$

$$V^{n'\sigma}_{nl_1\lambda'}(R) = \left\langle R_{nl_1}(r) \right| \frac{e^2 r_<^{\lambda'}}{r_>^{\lambda'+1}} \left| R_{n'\sigma}(r) \right\rangle ,$$

$$V^{nl_1}_{n'\sigma\lambda''}(R') = \left\langle R_{n'\sigma}(r) \right| \frac{e^2 r_<^{\lambda''}}{r_>^{\lambda''+1}} \left| R_{nl_1}(r) \right\rangle ,$$

$$V^{\infty\sigma}_{nl_1\lambda'}(R) = \left\langle R_{nl_1}(r) \right| \frac{e^2 r_<^{\lambda'}}{r_>^{\lambda'+1}} \left| F_\sigma(\eta, k_1 r) \right\rangle ,$$

$$V^{nl_1}_{\infty\sigma\lambda''}(R') = \left\langle F_\sigma(\eta, k_1 r) \right| \frac{e^2 r_<^{\lambda''}}{r_>^{\lambda''+1}} \left| R_{nl_1}(r) \right\rangle .$$

In the expressions for the V's, $r_<$ and $r_>$ refer to the lesser or greater of the scalar quantities r and R.

Equation (27) is the elastic channel Schrödinger equation for an electron scattering from a hydrogen atom in the nth excited state with eigenfunction $|R_{nl_1}(r)l_1m_1\rangle$. The parts of Eq. (27) which involve a sum from $n'=2$ to n'' and an integral from 0 to κ include all of the energy-conserving processes while the sum from n'' to ∞ and the integral from κ to ∞ represent projectile-target interactions which are closed by energy conservation.

If the target is initially in the ground state ($n=1$, $l_1=m_1=0$) then Eq. (27) assumes the simpler form

$$\left[-\frac{\hbar^2}{2\mu_p}\frac{d^2}{dR^2} + \frac{\hbar^2}{2\mu_p}\frac{l_2(l_2+1)}{R^2} - \frac{e^2}{a_0}\left(1+\frac{a_0}{R}\right)e^{-2R/a_0}\right]$$

$$\times U'(0l_2l_2|R) + \sum_{l=0}^{\infty} \sum_{\sigma=0}^{n'-1} \int K_{l\sigma}(R,R')$$

$$\times U'(0l_2l_2|R')R'\,dR' = 0 \;, \quad (28)$$

where a_0 is the radius of the first Bohr orbit and

$$K_{l\sigma}(R,R') = B_{l\sigma}\sum_{s=1}^{4} {}^{(s)}C_{l\sigma}(R,R') \;.$$

Here

$$B_{l\sigma} = \frac{1}{2\sigma+1}\,|\langle l_2\sigma 00|l0\rangle|^2 ,$$

where

$$\langle l_2\sigma 00|l0\rangle$$

is a vector coupling coefficient and

$${}^{(1)}C_{l\sigma}(R,R') = -\frac{2\mu_p iR}{\hbar^2} \sum_{n=2}^{n''} \beta_{n'} V^{n'\sigma}_{10}(R)\,j_l(\beta_{n'}R_<)$$

$$\times h_l^{(1)}(\beta_{n'}R_>)V^{10}_{n'\sigma}(R') ,$$

$${}^{(2)}C_{l\sigma}(R,R') = -\frac{4\mu_p R}{\pi\hbar^2} \sum_{n''}^{\infty} \alpha_{n'} V^{n'\sigma}_{10}(R)$$

$$\times i_l(\alpha_{n'}R_<)k_l(\alpha_{n'}R_>)V^{10}_{n'\sigma}(R') ,$$

$${}^{(3)}C_{l\sigma}(R,R') = -\frac{4\mu_p iR}{\pi\hbar^2} \int_0^{\kappa} \beta_c k_1^2 [V^{\infty\sigma}_{10}(R)\,j_l(\beta_c R_<)$$

$$\times h_l^{(1)}(\beta_c R_>)V^{10}_{\infty\sigma}(R')]\,dk_1 ,$$

and

$${}^{(4)}C_{l\sigma}(R,R') = -\frac{8}{\pi^2}\,\frac{\mu_p R}{\hbar^2} \int_{\kappa}^{\infty} \alpha_c k_1^2 [V^{\infty\sigma}_{10}(R)\,i_l(\alpha_c R_<)$$

$$\times k_l(\alpha_c R_>)V^{10}_{\infty\sigma}(R')]\,dk_1 \;.$$

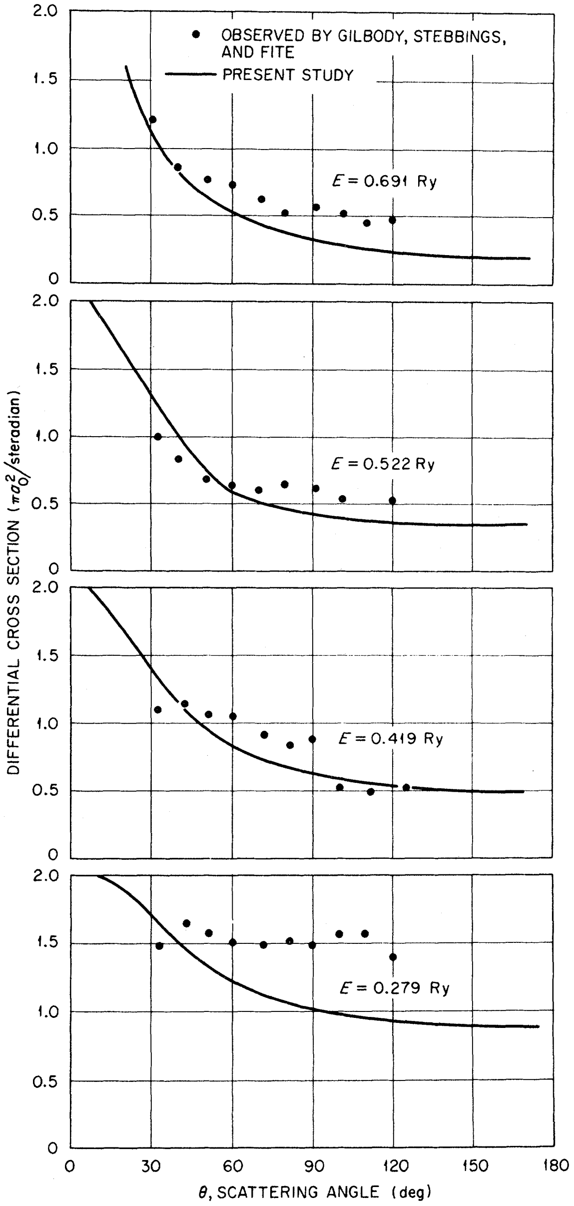

FIG. 1. Comparison of observed and calculated differential cross sections for electrons scattered by atomic hydrogen.

The V's are defined by the following expressions:

$$V_{10}^{n'\sigma}(R)=(V_{n'\sigma}^{10}(R))^{\dagger}=\left\langle R_{10}(r)\left|\frac{e^2r_<^\sigma}{r_>^{\sigma+1}}\right|R_{n'\sigma}(r)\right\rangle ,$$

$$V_{10}^{\infty\sigma}(R)=(V_{\infty\sigma}^{10}(R))^{\dagger}=\left\langle R_{10}(r)\left|\frac{e^2r_<^\sigma}{r_>^{\sigma+1}}\right|F_\sigma(\eta,k_1r)\right\rangle .$$

The scattering data presented in this study were obtained by numerically solving Eq. (28).

NUMERICAL PROCEDURES

We wish to generate the nonlocal potential $K(R, R')$ and solve the radial Schrödinger equation

$$\left(\frac{-\hbar^2}{2\mu_p}\frac{d^2}{dR^2}+W(R)\right)\psi(R)=\int_0^{R_m}K(R,R')\psi(R')\,dR' , \tag{29}$$

where

$$W(R)=E-\frac{\hbar^2}{2\mu_p}\frac{l_2(l_2+1)}{R^2}+\frac{e^2}{a_0}\left(1+\frac{a_0}{R}\right)e^{-2R/a_0} . \tag{30}$$

These relations describe an electron of energy E scattered from atomic hydrogen for all appropriate values of the relative-motion angular-momentum quantum number l_2. Here R_m is the radial distance beyond which the local potential $(e^2/a_0)(1+a_0/R)e^{-2R/a_0}$ is assumed to be negligibly small.

We wish to find the wave function ψ in the region $0 \leq R \leq R_m$ subject to the following boundary

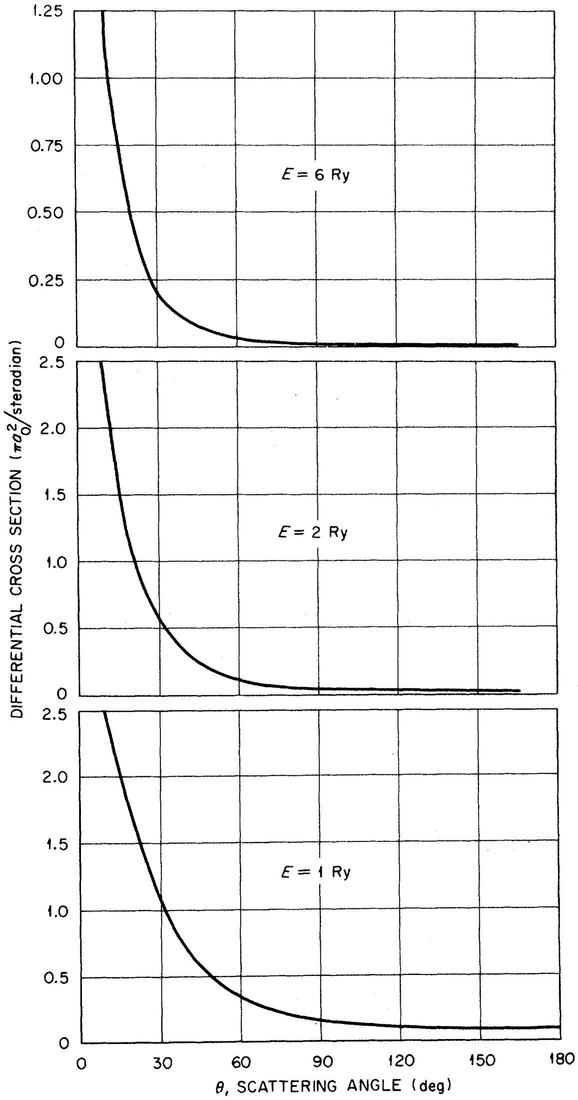

FIG. 2. Calculated differential cross sections for electrons scattered by atomic hydrogen.

conditions:

$$\psi(0)=0, \tag{31}$$

$$\psi(R_m)=\tfrac{1}{2}\left[h^{(1)*}(kR_m)+Sh^{(1)}(kR_m)\right], \tag{32}$$

and

$$\psi'(R_m)=\tfrac{1}{2}\left[h^{(1)*'}(kR_m)+Sh^{(1)'}(kR_m)\right], \tag{33}$$

where S is the scattering matrix element. The primes denote differentiation with respect to R.

The computer program used to solve Eq. (28) was written by Owen,[21] based on the method described by Robertson.[19] Discretizing Eq. (29) yields a set of simultaneous equations

$$\begin{aligned}\left(1+\tfrac{1}{12}d^2W_{i-1}\right)\psi_{i-1}-\left(2-\tfrac{5}{6}d^2W_i\right)\psi_i\\ +\left(1+\tfrac{1}{12}d^2W_{i+1}\right)\psi_{i+1}\\ =\tfrac{1}{12}d^2\sum_{j=0}^{N}\left(K_{i-1,j}+10K_{ij}+K_{i+1,j}\right)T_j\psi_j,\\ i=2,3\cdots N.\end{aligned} \tag{34}$$

Here d is the interval size and T_j is the weighting appropriate for Simpson's rule. There are only $N-1$ simultaneous equations since ψ_0 is fixed by the boundary condition (31) and ψ_1 is arbitrarily chosen. The solution to Eq. (34) may be renormalized to satisfy the boundary conditions (32) and (33). Equation (34), which is of order d^4, is solved by Gaussian elimination with partial pivoting.[20] Results of timing and accuracy tests on this code are given by Reeves and Owen.[21]

Both the nonlocal potential generator routine and the code for solution of the Schrödinger equation were written in double precision FORTRAN IV. A typical run, involving generation of the nonlocal potential for a single projectile energy and solution of the resulting Schrödinger equation, requires less than 8 min on the IBM 360/91 computer.

VI. RESULTS AND DISCUSSION

The computer code [used in the solution of Eq. (26)] was written in a versatile manner. Effects produced by the real and imaginary parts of the kernel, $K(R, R')$, can be examined independently or simultaneously. The structure of the kernel also allows one to consider separately the bound and continuum states of the target.

Comparison between our calculated results and those observed experimentally by Gilbody, Stebbings, and Fite[22] are shown in Fig. 1. With the exception of 0.279-Ry measurements, we find good agreement. The disparity between our theoretical and the measured results at 0.279 Ry may be attributable to increased experimental difficulties at this low energy. Examples of calculated angular distributions for electron energies greater than the excitation or ionization thresholds are shown in Fig. 2.

Comparisons between the data of Brackmann, Fite, and Neynaber[23] (obtained from the p-wave calculations of McEachran and Frazer[24]) and those of Neynaber, Marino, Rothe, and Trujillo[25] are shown in Fig. 3. Our results agree remarkably well with both sets of these data over the energy range in which the measurements were made. The importance of the distortion effect is readily seen in the difference between the calculated and static elastic scattering cross sections. According to these results, the adiabatic approximation is poor in the energy range considered here.

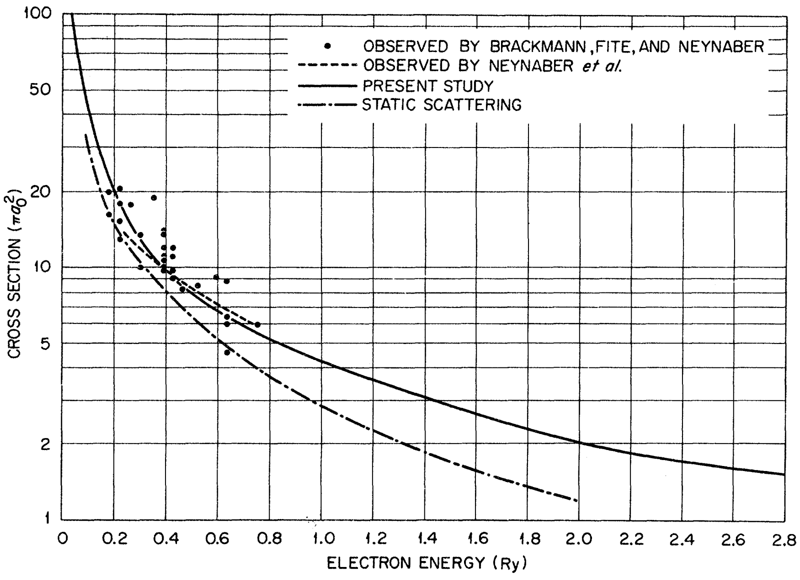

FIG. 3. Comparison of observed and calculated elastic cross sections for electrons scattered by atomic hydrogen.

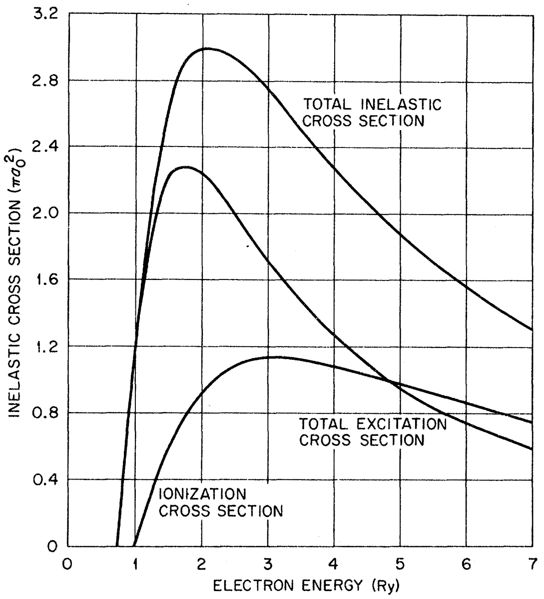

FIG. 4. Calculated total excitation, ionization, and total inelastic cross sections for electron collisions with atomic hydrogen.

In Fig. 4 we show the total discrete excitation, ionization, and total inelastic cross sections. Excited states through $n = 10$ were included in the discrete parts of the kernel, $K(R, R')$, this level having an excitation energy within 1% of ionization. The individual inelastic cross-section curves were obtained by including the discrete and continuum parts of the kernel separately. Therefore, the excitation and ionization values shown in Fig. 4 are approximate. The errors introduced by considering the discrete and continuum states of the target separately are not very great as can be seen by comparing the sum of the individual cross sections with that for total inelastic scattering. The results represented by the latter curve were obtained by including all of the inelastic processes simultaneously. The maximum in the total inelastic cross section occurs at 2 Ry while that for the total excitation occurs at 1.7 Ry. The ionization cross section is equal to the total excitation cross section at 5 Ry and becomes the dominant factor in the inelastic scattering processes at higher energies.

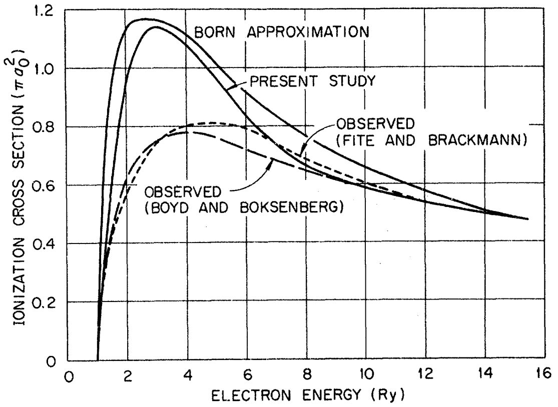

FIG. 5. Comparison of observed and calculated cross sections for ionization of atomic hydrogen by electron impact.

Comparison of the calculated ionization cross section with the experimental measurements of Fite and Brackmann[26] and Boyd and Boksenberg[27] are shown in Fig. 5. Our curves agree in general shape and energy at which the observed maximum occurs. The fact that the calculated results are

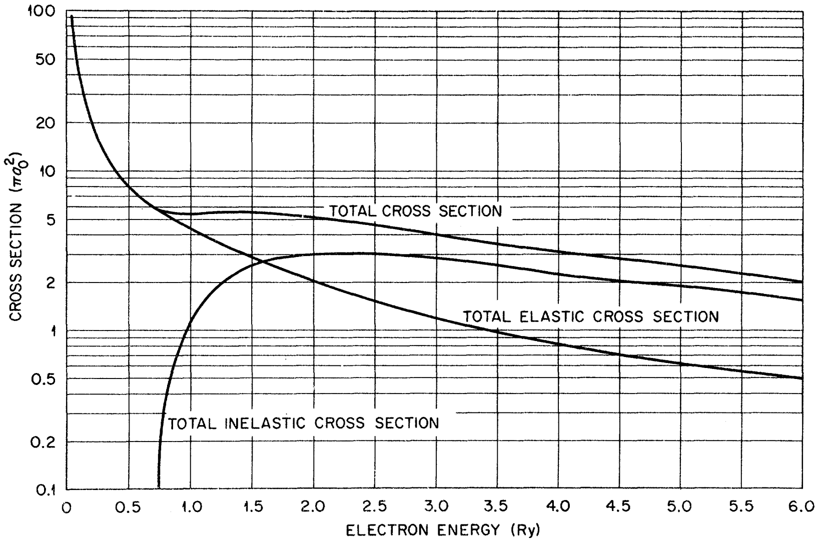

FIG. 6. Calculated total elastic, inelastic, and total cross sections for electron collisions with atomic hydrogen.

higher than those observed may be indicative of the importance of exchange in the ionization process or perhaps the approximations made in our model.

The total elastic, inelastic, and interaction cross sections are shown in Fig. 6.

VII. CONCLUSIONS

In this study we have incorporated in a consistent manner all of the significant contributing open channels to the scattering of slow electrons from atomic hydrogen. We have demonstrated that the zeroth-order approximation made in the exact Green's function yields results which agree well with the available data. Obviously, physically more realistic approximations can be made which are tractable—some of which were suggested in Sec. III. For practical reasons these approximations preclude incorporation of the continuum contributions to the optical potential.

The present model could be improved by including exchange into the formalism. However, this would introduce additional nonlocality into the model, and it is not certain what numerical difficulties would result.

We have omitted the bound- and resonance projectile-state contributions. These closed-channel terms contribute principally to the real part of the optical potential and, consequently, affect the elastic scattering process below the first excitation level. The resonances arise as a result of formation of negative-ion states at energies near the discrete excitation threshold. These states are unstable toward autodetachment and are usually a few tenths of an electron volt in width. In hydrogen, one permanently bound negative-ion state has been observed and has a measured binding energy of 0.8 eV.[28,29] The formation of such a state must involve a third body—either another electron, photon, or hydrogen atom. The significance of such processes in elastic scattering of electrons from atomic hydrogen is not expected to be important.

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[1] The close-coupling method has been studied extensively in applications to simple atomic systems. The successes and limitations of this technique in determinations of elastic and inelastic scattering phenomena have been summarized recently by P. G. Burke [Comments At. Mol. Phys. 1, 35 (1969); and in *The Physics of Electronic and Atomic Collisions*, edited by L. M. Branscombe (Joint Institute for Lab-Astrophysics, University of Colorado, Boulder, 1968).

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